# Constraining Least-Squares VLBI Solutions

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**Abstract** In a traditional least-squares adjustment of parameters to the Very Long Baseline Interferometry (VLBI) observations, typically tropospheric as well as clock parameters are determined in the form of continuous piece-wise linear functions with a given temporal resolution. As the VLBI observations are not equidistant, but on the contrary exhibit gaps of sometimes several hours, singularities arise due to unresolvable parameters inside these gaps. For this reason, it is common practice to constrain the respective parameters in the solution. In this paper we analyze the singularities that arise within the geodetic VLBI data analysis by means of a Singular Value Decomposition of the Jacobian matrix. Furthermore, we show the ramifications of traditional constraining. Finally, we present an alternative approach for optimizing the least-squares solution by omitting the constraints within the VLBI solution and performing a Tikhonov regularization. In this way, we obtain a minimally regularized solution, which leads to reliable target parameters without being influenced by constraints on auxiliary parameters such as clocks or troposphere.

**Keywords** VLBI, least-squares adjustment, constraints, Tikhonov regularization

## 1 Introduction

Geodetic Very Long Baseline Interferometry (VLBI) observations are used for the determination of fundamental geophysical parameters, such as, e.g., Earth orientation parameters (EOPs), as well as the celestial and terrestrial reference frames (CRF and TRF). This parameter estimation is typically done in a classical least-squares adjustment. Together with the mentioned target parameters, auxiliary parameters have to be estimated with high temporal resolutions even below one hour. In most cases, these are parameters for clock synchronization as well as tropospheric parameters.

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In a routine parameter estimation process, a single solution set-up is chosen to process a lot of VLBI sessions. Unfortunately, not all sessions permit estimation of the entire set of parameters, leading to instabilities of the least-squares solution, which are typically cured by adding constraint equations, whether needed or not. Basically, there are two reasons for these singularities. On the one hand, radio telescopes might miss observations due to various reasons, e.g., too strong winds; data gaps of up to several hours can appear. On the other hand, some observing network geometries are not sensitive for all of the parameters.

Even in the next generation VLBI Global Observing System (VGOS, [4]) era, where large global networks will operate with high data rates, the constraining still might be an issue. Especially, when automatic processing is considered due to the huge number of observations, this will become a crucial point which has to be handled with care.

## 2 Least-Squares Adjustment and Diagnosis by Singular Value Decomposition

In most of the VLBI analysis packages, an ordinary least-squares approach [3] is chosen to estimate the necessary parameters $\mathbf{x}$ from the observations $\mathbf{b}$. The basic idea of the least-squares adjustment is to minimize the sum of the squared residuals $\mathbf{r}$ to deal with the overdetermined linear or linearized equation system

$$\mathbf{b}+\mathbf{r}=\mathbf{A}\mathbf{x} \tag{1}$$

where the matrix $\mathbf{A}$ represents the linear(ized) relationship between observations and parameters, i.e., the Jacobian matrix $\mathbf{A}=\partial\mathbf{b}/\partial\mathbf{x}$. In other words, a solution has to be found, where the gradient of the residuals vanishes. This directly leads to the solution via the normal equations

$$\mathbf{x}=\left(\mathbf{A}^T\boldsymbol{\Sigma}_{bb}^{-1}\mathbf{A}\right)^{-1}\mathbf{A}^T\boldsymbol{\Sigma}_{bb}^{-1}\mathbf{b}, \tag{2}$$

where a weighting is included based on the inverted covariance matrix of the observations $\boldsymbol{\Sigma}_{bb}$.

Applying a Cholesky decomposition [1] on the weight matrix

$$\boldsymbol{\Sigma}_{bb}^{-1}=\mathbf{R}^T\mathbf{R}, \tag{3}$$

leads to a full de-correlation and, thus, to a modified Jacobian matrix and observation vector

$$\mathbf{X}=\mathbf{R}\mathbf{A}, \qquad \boldsymbol{\xi}=\mathbf{R}\mathbf{b} \tag{4}$$

$$\Rightarrow \quad \mathbf{x}=\left(\mathbf{A}^T\mathbf{R}^T\mathbf{R}\mathbf{A}\right)^{-1}\mathbf{A}^T\mathbf{R}^T\mathbf{R}\mathbf{b} \tag{5}$$

$$=\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}\boldsymbol{\xi}. \tag{6}$$

Finally, a Singular Value Decomposition (SVD, [1]) of the transformed Jacobian matrix can be performed

$$\mathbf{X}=\mathbf{U}\mathbf{S}\mathbf{V}^T \tag{7}$$

leading to a new representation of the solution [1]

$$\mathbf{x}=\sum_i\frac{\mathbf{u}_i^T\boldsymbol{\xi}}{s_i}\mathbf{v}_i. \tag{8}$$

Obviously, problems arise if (numerically) zero singular values $s_i$ exist, because in this case the null space of the Jacobian matrix does not disappear, i.e., some parameters are not indeterminable. Thus, the SVD can be used as a tool to diagnose the numerical stability of the solution. If a singular value $s_i$ is numerically zero, the largest entries of the corresponding right singular vector $\mathbf{v}_i$ indicate weakly or undefined parameters. Furthermore, this singular vector is a base vector of the null space.

## 3 Effects of Standard Constraints

Typically, a stabilization of the least-squares adjustment can be achieved by constraining the solution, i.e., by adding some pseudo-observations which have sufficient information in the null space. Thus, a constraint matrix $\mathbf{C}$ with corresponding standard deviations can be constructed and added to the normal equations (Eq. 2)

$$\mathbf{x}=\left(\mathbf{A}^T\boldsymbol{\Sigma}_{bb}^{-1}\mathbf{A}+\mathbf{C}^T\boldsymbol{\Sigma}_{cc}^{-1}\mathbf{C}\right)^{-1}\mathbf{A}^T\boldsymbol{\Sigma}_{bb}^{-1}\mathbf{b} \tag{9}$$

as the constraints and the original observations are uncorrelated and the actual pseudo-observations are zero. If the solution should be solved and analyzed by means of SVD, the constraining can be equally achieved by extending the corresponding matrices and vectors

$$\mathbf{A}=\begin{pmatrix}\mathbf{A}\\ \mathbf{C}\end{pmatrix},\ \mathbf{b}=\begin{pmatrix}\mathbf{b}\\ \mathbf{0}\end{pmatrix},\ \boldsymbol{\Sigma}_{bb}=\begin{pmatrix}\boldsymbol{\Sigma}_{bb} & \mathbf{0}\\ \mathbf{0} & \boldsymbol{\Sigma}_{cc}\end{pmatrix}. \tag{10}$$

It is important to note that the constraints do not have to be the basis of the null space. They only need to have components in the null space.

In routine VLBI data analysis, three types of constraints are relevant. These are offset constraints, rate constraints, and no net translation/no net rotation conditions to define the geodetic datum. In this paper, we focus on offset constraints which force a parameter to be zero where a column of the constraint matrix has the form

$$\mathbf{C}_i=\begin{pmatrix}0 \dots 0\ 1\ 0 \dots\end{pmatrix}.$$

Furthermore, rate constraints

$$\mathbf{C}_i=\begin{pmatrix}0 \dots 1\ -1\ 0 \dots\end{pmatrix}$$

are investigated, which force the difference between two parameters to be zero. To overcome the datum deficiency, station and quasar positions are simply not estimated. Thus, only the EOPs are estimated as well as clock parameters (quadratic polynomial and continuous piece-wise linear functions (CPWLF) with a resolution of 1 *h*), zenith wet delays (ZWDs, 1 *h* CPWLF), and tropospheric gradients (1 *d* CPWLF). All auxiliary parameters are set up per station; however, the clock parameters for one station need to be fixed to realize a reference.

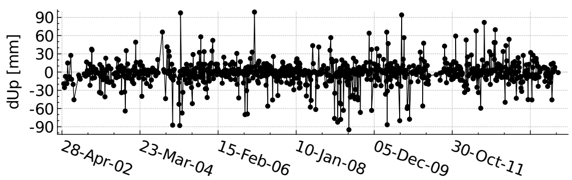


**Fig. 1** Height differences for the station TIGOCONC with two different weights for the troposphere constraints. Note that larger differences (> 100 mm) are excluded.

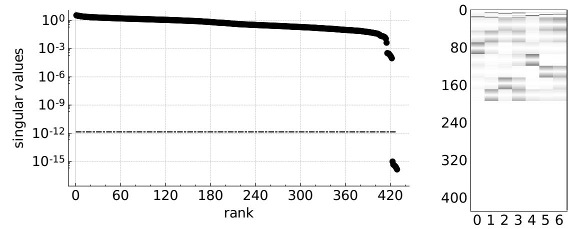


**Fig. 2** Singular values (left) and null space of the Jacobian matrix (right). The rank deficiency of seven is related to eight sessions in this experiment, and the basis vectors of the null space are dominated by clock polynomial parameters (one station is the reference station).

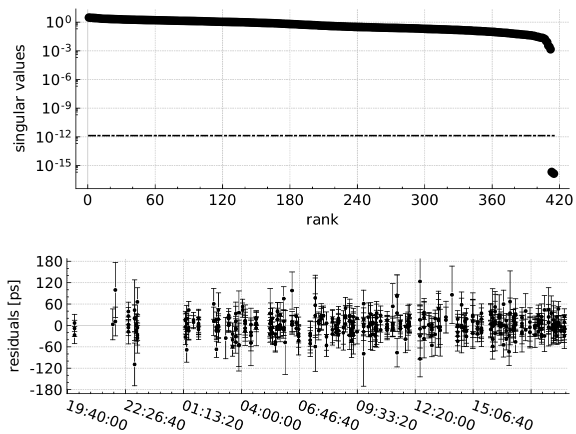


**Fig. 3** Singular values (top) for the session 02OCT16XA and the residuals for ALGOPARK from the standard solution (bottom) representing the temporal distribution of the observations.

In mass processing of VLBI sessions (batch solutions), a set of offset and rate constraints are always applied regardless of whether the null space of the Jacobian matrix exists or not. Thus, often constraining information is added although it is not necessary. To evaluate this procedure, we performed two different solutions:

1. with standard constraints
   - $\sigma_{ZWD_{rate}} = 40$ ps/h
   - $\sigma_{grad_{offset}} = 1$ mm, $\sigma_{grad_{rate}} = 2$ mm/d
   - $\sigma_{clock_{rate}} = 10^{-14}$
2. with modified weights for the constraint equations
   - $\sigma_{ZWD_{rate}} = 10$ ns/h
   - $\sigma_{grad_{offset}} = 0$ mm, $\sigma_{grad_{rate}} = 0$ mm/d
   - $\sigma_{clock_{rate}} = 10^{-14}$

for VLBI sessions between 2000.0 and 2016.0. With the modified set-up, about 15% of the solutions failed, indicating that the constraints have been necessary. However, for the other sessions differences appear up to the decimeter level (see Figure 1). Even for the currently best VLBI dataset from the continuous VLBI campaign 2014, height differences of up to 7 mm appear (not shown here) indicating that the effects are also relevant in the VGOS era. However, it has to be noted that the differences are typically not significant when compared to the standard deviations of the parameters.

## 4 Development of an Alternative Approach

When investigating the least-squares solution without any constraint, always a rank deficiency is present. As can be seen in Figure 2, the null space of the Jacobian matrix is dominated by the linear and quadratic clock polynomial parameters. Thus, eliminating the clock polynomials from the functional model of the least-squares solution leads to a regular solution for a well-observed session. In this case, a solution without any constraints leads to a reasonable result with a weighted root mean squared (WRMS) post-fit residual of 27.2 ps, which is 0.3 ps below the WRMS of the standard constrained solution with full clock set-up. However, for another session the approach fails (see Figure 3) due to observation gaps for the station ALGOPARK. These gaps lead to an over-parameterization and, thus, to a singularity. However, none of the parameters are entirely undefined. As a consequence, simply dropping individual parameters is not a feasible approach.

Unfortunately, for this session there are a few observations in every parameterization interval causing a

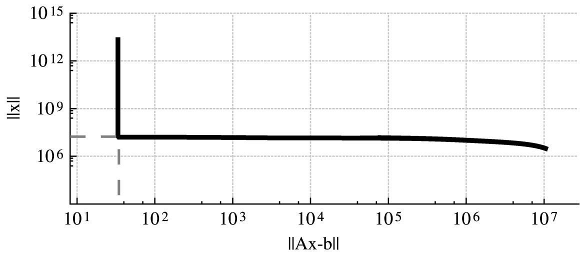


**Fig. 4** L-curve, i.e., plot of the solution norm w.r.t. residual norm, which is used to determine the regularization parameter depending on the solution representing the corner.

bad condition of the least-squares problem. To overcome this without the need for constraining, a regularization can be performed. Here, the Tikhonov regularization [5] has been chosen, where the squared parameter norm is minimized in addition to the squared residual norm

$$\min_x \left\{ \|\mathbf{Ax}-\mathbf{b}\|_2^2 + \lambda^2 \|\mathbf{x}\|_2^2 \right\}. \tag{11}$$

The Tikhonov parameter $\lambda$ is considered to balance between smoothing the estimates and minimizing the residuals. In the actual solution, the regularization parameter is used to filter out the impact of the small singular values

$$f_i = \frac{s_i^2}{\lambda_i^2 + s_i^2}, \tag{12}$$

$$\mathbf{x}_{filtered} = \sum_{i=1}^{n} f_i \frac{\mathbf{u}_i^T \boldsymbol{\xi}}{s_i} \mathbf{v}_i. \tag{13}$$

Thus, the singularity of the initial approach is eliminated. However, the choice of $\lambda$ is crucial for the success of this approach.

There are various possibilities for choosing the Tikhonov parameter. We make use of the so-called L-curve [2] (see Figure 4), which is a plot of the size of the regularized solution versus the size of the corresponding residual norm for all valid regularization parameters. To obtain this curve, 200 solutions are performed where the minimal and the maximal $\lambda$ are chosen according to the singular values

$$\begin{aligned} \lambda_{min} &= \max[s_{min}, \varepsilon \cdot s_{max}] \\ \lambda_{max} &= s_{max} \end{aligned} \tag{14}$$

with a tiny value $\varepsilon$, which is sixteen times the next positive representable value after zero. The optimal regularization is the one in the lower left corner of the L-shape as this represents minimal smoothing of the parameters and minimal residual norm.

This procedure, i.e., a totally unconstrained solutions with hourly clocks and ZWDs as well as daily tropospheric gradients and the full set of EOPs, has been applied to the continuous VLBI campaign 2002. For sessions where rank deficiencies appear, parameters without any observations have been eliminated. If further ill-conditioning has been present, the Tikhonov regularization parameter has been determined from the L-curve and used for the regularized solution. The resulting UT1–TAI time series is depicted in Figure 5. Slight differences can be seen between our new solution and the standard approach. However, these are only indirect changes of one of the target parameters due to modified handling of the auxiliary parameters.

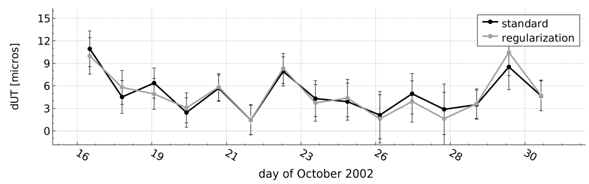


**Fig. 5** UT1–TAI for the standard (black) and the new regularized approach without constraints (gray).
In Figure 6 the effects on ZWDs are shown. On the one hand it can be noted that fixing the clock polynomials has only a minor effect on the ZWDs.

This step is one of the necessary changes of our new approach, as it eliminates extremely high correlations between the clock parameters and, thus, allows for neglecting the constraint equations. On the other hand it can be seen from Figure 6 that the parameters which are affected by the regularization have no physical meaning as they are far too large. However, they can easily be declared as outliers if ZWDs should be investigated. Thus, the new approach can be considered successful as no constraints are necessary for the regularized solutions. The resulting time series of target parameters are, therefore, not influenced by model assumptions.

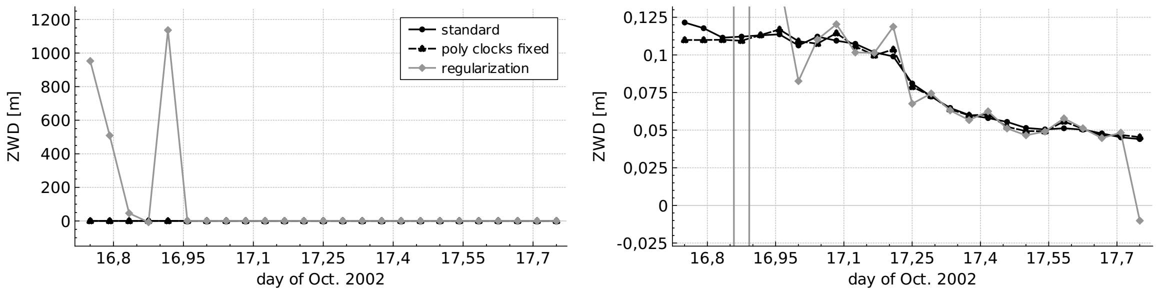


**Fig. 6** ZWDs for the standard solution (black circles), a solution without clock polynomials but with constraints (black triangles w/ dashed lines) and the new regularized approach without constraints (gray diamonds). The entire times series (left), clearly shows the outliers for regularized parameters. The zoom to a reasonable range of the parameters (right), however, shows that the other parameter estimates are resonable.

## 5 Conclusions

We analyzed the effect of routinely applied constraint equations in VLBI data analysis. The reason for these constraints, which are usually applied in the form of pseudo-observations weighted by standard deviations, are implied to overcome deficiencies in the solution set-up. For instance, the observing geometry might not allow for estimating tropospheric gradients if the local hemispheres above any telescope are not regularly sampled. Furthermore, gaps in the observations can lead to some over-parameterization.

We have shown that changing the standard deviations of the tropospheric parameters can lead to station position changes at the cm-level. Even for the currently most precise set of observations from the continuous VLBI campaign 2014, changes of the station positions of up to 7 mm have been detected.

Furthermore, we demonstrated that it is not possible to simply remove the constraints even for sessions where almost perfect data distribution is given. The reason is the set-up for the clock synchronization where second degree polynomials are estimated simultaneously with CPWLF leading to high mathematical correlations. By removing the clock polynomials, still a reasonable solution can be derived. Subsequently, it is possible to eliminate all constraint equations if the data distribution is homogeneous over a session. If this is not the case, still rank deficiencies appear. With our modified solution approach implementing the Tikhonov regularization we, however, are able to deal with such situations without applying constraints. In this way, we derive time series of target parameters that are not influenced by model assumptions. Parameters which are strongly affected by the filtering process as they represent the null space of the Jacobian matrix are derived with unrealistic estimates. However, these could be handled as outliers in, e.g, an analysis of ZWDs.

Thus, we presented a new approach for geodetic VLBI data analysis. This approach is not based on any constraint equations and, therefore, permits a set-up for the VGOS era where the equation system is stabilized only in situations where it is necessary.

## References

1. J. W. Demmel (1997) Applied numerical linear algebra. Siam. Philadelphia.
2. P.C. Hansen (1999) The L-curve and its use in the numerical treatment of inverse problems. IMM, Department of Mathematical Modelling, Technical University of Denmark.
3. K.R. Koch (1999) Parameter Estimation and Hypothesis Testing in Linear Models, vol 2., upd. and enl. ed. Springer, Berlin; Heidelberg; New York; Barcelona; Hong Kong; London; Milan; Paris; Singapore; Tokyo.
4. A. Niell., C. Beaudoin, R. Cappallo, B. Corey, M. Titus (2013) First results with the GGAO12M VGOS System, *In: Proceedings of the 21nd European VLBI Group for Geodesy and Astrometry Working Meeting*, Helsinki, Finland, Reports of the Finnish Geodetic Institute, ISBN: 978-951-711-206-3, 217–221.
5. A. Tikhonov, V.Y. Arsenin (1977) Solutions of ill-posed problems. 1977. Wiley, New York.